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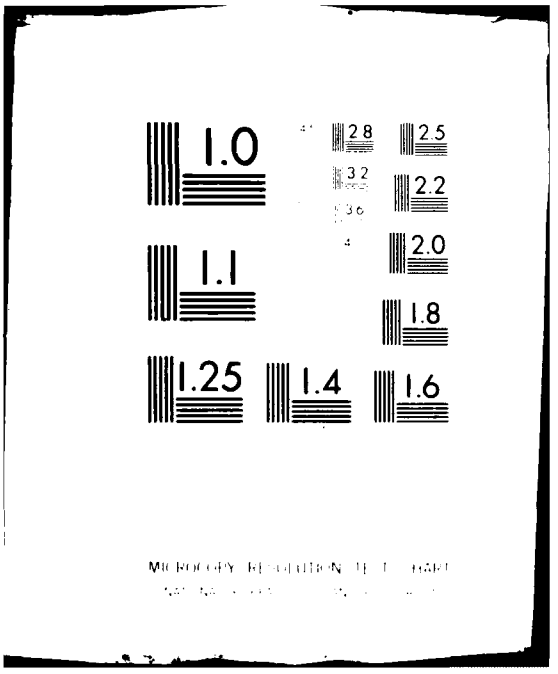
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NON-LINEAR LEAST CHI-SQUARE ALGORITHM
AN IMPROVEMENT ON NON-LINEAR LEAST SQUARES

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Introduction. Because of the high cost of testing, many large weapon systems cannot be tested over the full range of possible battlefield parameters. As a result, the developer and the reviewing authorities have come to rely on system simulation to demonstrate the system capability over the range of untested parameters. These simulations also are useful to investigate the change in performance resulting from possible subsystem modifications. In some important programs, the Government relies on simulations of competing systems to indicate the relative performance of these systems in situations for which no tests have been made, although of course, simulations such as these have been validated as much as possible by system tests. In these instances the procurement decision rests heavily on the validity of the system simulations. Consequently the need arises for a generally accepted procedure which is undoubtedly fair to each contractor and provides the maximum amount of objective judgment about the validity of the simulation. In any such procedure the Government must be able to rapidly evaluate simulations furnished from a variety of sources.

The procedure must be workable and economical -- that is it must apply a lot of leverage to the problem with regards to manpower, -- computer programmers and engineers -- the cost, -- computer running time and validation experiments -- and elapsed time. Implicit in this discussion is that planning for system simulation validation must be completed before the first system RFQ is issued.

Many methods are used for system simulations: Monte Carlo, analog, hybrid, and digital simulation of differential equations. A variety of special and general purpose programs are available for the simulator's use. Among then are "SPERT", "ACSL," and HIT PRO." The problem for the user of these simulations comes when he needs to compare theory with experiment and asks the questions: How good is the theory? Is

the agreement between theory and experiment good enough to validate the simulation? (As an example of these questions see Pastrick (1, 2).) Another question to be considered is: Could it be that the experiment was defective in any way?

Many simulations have not been prepared in such a way so that they can be used to answer these questions. In the first place, the simulations are not designed to adjust parameters to fit data. In the second place, the system itself may be so complex that the computing time for complete system simulation is so long that adjusting the parameters to achieve a better fit between simulation and experiment is not feasible. Thus a new procedure is needed to combine theory and experiment.

The procedure suggested by this paper is the use of the least chi square computer program to simulate the major subsystems of a system simulation and validate it against test data.

Criteria for comparison, and iteration procedure. In fitting data to non-linear models of system performance such as systems of differential equations, the usual criteria is the iterative minimization of the sum of the squares of the residuals. Other criteria, such as generalized least squares have also been considered and demonstrated (3). As Aitken (4) noted with respect to generalized least squares, the criteria to be used are a matter of choice. In other words, we are free to decide whether least squares is the best criteria for our purpose. A particular concern with the ordinary least squares procedure is whether the residuals are consistent with being drawn from a random sequence.

Many tests have been devised (5) for this purpose. One test of special interest in this paper is the Box-Pierce (6) test which is the sum of the squares of the autocorrelation coefficients divided by their variances. A typical term is $(r_i)^2 v_i^{-1}$.

Given all these tests, no way had been devised to adjust the parameters to better satisfy the data until it was proposed that this criteria be combined with least squares to obtain a new criteria: least chi-square (Moore, 7, 8, 9). By finding the parameters which minimize chi-square, the probability is maximized that the residuals come from a population with a given variance σ_e^2 , and from a random sequence. The variance must be independently determined from theory or measurement as the measurement error.

Thus, a probability can be generated from the computed chi-square which permits the statistician and decision-maker to compare the "goodness of fit" of the simulation of several quite different systems. In this way a direct comparison of the validity of the simulations can be made.

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The figure of merit, χ^2_{TW} (chi-square total) is the sum of χ_1^2 and χ_2^2 , the Box-Peirce number $\{\sum_j v_j^{-1}(\sum_i^n d_i d_j)/\sum d_i^2\}$

Derivation: We will follow the procedure and most of the notation of Aitken (4) for generalized least squares:

Let the representation of the vector of data:

$$u = (u(x_1), u(x_2), \ldots u(x_n))$$

by the theoretical vector, be:

$$y = (y(x_1), y(x_2), \ldots y(x_n))$$

$$u_i^* = u_i - y_i^* .$$

Let θ^* denote a column vector of k + 1 coefficients independent of y such that:

$$\theta^* = (\theta_1^*, \theta_2^*, \theta_3^*, \ldots \theta_{k+1}^*)$$

Define the matrix P* as the matrix whose ith row is

$$\frac{\partial y_i^*}{\partial \theta_1} , \frac{\partial y_i^*}{\partial \theta_2} \cdots \frac{\partial y_i^*}{\partial \theta_r}$$

(The asterisk symbol * will be used to indicate an estimate of the indicated sysbol where convenient. However, it will not be used on complex expressions involving χ^2_T, σ^2, and r_j because of typographical difficulties).

In this expression V_j^{-1} is defined as follows:

$$V_1^{-1} = \begin{bmatrix} 0\,1\,0 \ldots 0 \\ 0\,0\,1\,0 \ldots 0 \\ 0\,0\,0\,1\,0 \ldots 0 \\ \ldots \end{bmatrix}; V_2^{-1} = \begin{bmatrix} 0\,0\,1\,0 \ldots 0 \\ 0\,0\,0\,1 \\ 0\,0\,0 \end{bmatrix} \qquad V_j^{-1} = \begin{bmatrix} 0\,0 \ldots 0\,1 \ldots \\ 0\,0\,0 \ldots \ldots 0\,1 \ldots \\ \ldots \end{bmatrix}$$

In these, the subscript "j" indicates a unit value in each of the ith rows and (i + j)th column.

If v_j is the variance of r_j , then

$$\chi_T^2 = \sigma_0^{-1} d'd + \sum_{j=1}^{s} r_j^2 / v_j$$

and: $r_j = d' V_j^{-1} d / (dd')$

(Note the difference between V_j^{-1} and v_j^{-1}.

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On differentiating (χ_r^2) with respect to (θ^*) and substituting

$$(d^*) = P^* [\delta\theta^*] - u^*.$$

as an estimate of the increment of the residuals needed to minimize χ_r^2 , the algorithm for $[\delta\theta^*]$ becomes:

$$[\delta\theta^*] = [P^{*\prime} \Gamma P^*]^{-1} P^{*\prime} \Gamma u^*.$$

WHERE:

$$a_j = \frac{2r_j V_j^{-1}}{(d)'(d)/\sigma_e^2 - 2\sum_{i=1}^{s} (r_i)^2 V_i^{-1}}$$

$$\Gamma = I + \sum_{i=1}^{s} a_i r_i V_i^{-1}$$

If Γ equals I, the expression for $[\delta\theta^*]$ reduces to $[P^{*\prime}P^*]^{-1} P^{*\prime} u^*$, which is the same as the algorithm for ordinary non-linear least squares used in such computer programs as provided by both IBM and CDC libraries as well as in SAAM-27.

By inspection, $P^* \Gamma$ replaces $P^{*\prime}$ in the ordinary expression. To modify the ordinary expression, Γ is computed. P*' is postmultiplied by Γ , and the product placed in the computer memory where P*' is normally stored. χ_r^2 is substituted for dd' whereever it occurs and no further change is need in the iteration procedure.

These expressions have been programmed into the Simulation And Analysis Modeling (SAAM-27) program of Berman et al, (10, 11) as indicated above, multipying P*', by Γ , and letting the program proceed from that point. The usual iteration continues. The computer program resulting from this change has been designated for control purposes as SAACH, and has been tested on the CDC 6600 at ARRADCOM, Dover, to determine the following questions:

1. How much change is there in the final parameter estimates?

2. What change, if any, is there in the number of iterations?

3. What change is there in the time per iteration?

Four problems of different origin and which use different mathematical models have been run on the SAACH program to answer the above questions. In the first example: Gun Chamber Pressure Waves, the mathematical model used is the superposition of two pressure waves generated by analytic models in the program, with the adjustment of up

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to eight parameters to obtain the best fit to observed data. In the second example, an aircraft control system simulation, the mathematical model is a set of four linear differential equations, simulating the Yaw Damper system on an aircraft. These equations were solved by a special procedure developed for SAAM-27 by Berman et al. (12), with up to four adjustable parameters. In the third example, a biomedical problem furnished as a test case by Miss Rita Straub of Brookhaven National Laboratory, the mathematical model was a set of seven coupled linear differential equations with five adjustable parameters; this was solved by the same method as used in the second case. In the fourth and final example: KEWB Kinetics, a simulation of the nuclear reactor transients of the Kinetic Experiment Water Boiler, the mathematical model was an extremely non-linear set of coupled differential equations as described by Hetrick and Gamble (13). These equations were integrated by the fourth order Runge-Kutte integration procedure of SAAM-27, with only one adjustable parameter. The results of these analyses were discussed in detail at the 1979 Design of Experiments Conference (9). Abbreviated discussions of the result of each problem follow.

Gun Chamber Pressure Waves. Unusual pressure waves suggestive of an acoustic wave superposed on the normal gun chamber pressure-time curve, have occurred in tests of the XM211 propellant charges at zone 3 for the M101 projectile in the 155mm gun, (Knutelski, (14)). The mathematical model used was:

$$P = P_1 \exp\{-(t-t_1)^2/2\sigma_1^2\} + P_2 \exp\{-(t-t_2)^2/2\sigma_2^2\} \times \sin\{2\pi f (t-t_3) + \pi/2\}$$

Three parallel cases were computed once the fit was good enough to permit iteration with different ranks of autocorrelation. Because of computing difficulties which arose when trying to converge on six or seven parameters, the iteration was initially restricted to four parameters: Once the fit was good and had converged using these four parameters, their final values were used as initial values for a six-parameter fit. Finally, all eight parameters were allowed to vary.

Two results of this series of analysis are plotted in Figs 1, and 2. The case numbers are BGK-3.30356301-0, and 3.30356511-5. The first has no autocorrelation coefficients; the second, 5, a third, (not shown), 10. The parameters for these cases are given in Table 1, (note that the last three digits only of the identifier are used here). Some parameters are quite different from case to case.

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The apparent fit from the figures is best for the case of five autocorrelations given in Fig. 2. The fit of this case was also better than that for 10 autocorrelations which is not illustrated.

The value of the sum of the squares of the residuals as shown in Table 1 was actually much smaller for cases 511-10, and 301 than for 511-5 yet the fit as noted above was not as good.

The last row of Table 1, gives the values of σ_b^2, the experimental variances assumed for these cases. These were arbitrary numbers taken as example only, because the precision of the measurement system is probably much greater than the value given; i.e., the variances should be smaller. However, if smaller values were used, such as when case 511-10 is compared to 511-5, the weight on the sum of the squares is greater but the goodness of fit appears to decrease, thus illustrating the need for least chi-square iteration.

Table 1 also shows the effect of least chi-square in terms of number of iterations, and computing time. When five autocorrelations were used, as in case 511-5, only a small increase in number of iterations is found and a moderate increase in computing time as compared to 301. If ten autocorrelations were used, as in 511-10, the number of iterations increased, and the time increase was 1.8 times greater, giving about double the increase in time for double the number of autocorrelation coefficients.

Table 2 shows the autocorrelations up to order 20 for the three cases. The values of X_1^2, X_2^2, and X_3^2 for the number of autocorrelations used (0, 5, 10) is shown in the last rows of this table.

Aircraft Control Systems. A typical aircraft yaw damper design problem (15), was analyzed to illustrate the use of least chi-square. To optimize the design, four parameters may be adjusted to give the best fit to a desired response curve. These parameters are K_0, K_4, τ, and δ. These correspond to the parameters L(0,4), L(4,1), L(4,1), L(4,2) and L(4.3). A vector of a random sequence of normally distributed errors from a population with variance of $(.033)^2$ was added to the data vector to simulate the effects of sampling error; this may be considered to represent an allowable error or tolerance in fitting the curve.

The value of was set at $(.033)^2$, six autocorrelations were used for the problem which was identified as CONRLM 4.011-6. Another run was used on the same data with the standard least squares algorithm. Fig. 3 shows the fit obtained for the data and is typical of the results. Table 3 showns the number of iterations for each case. It took 4 iterations for the ordinary algoithm to converge, and only two for the least chi-sqare algorithm with six autocorrelation coefficients (CONRLM 4.011-6).

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UNITS	SYMBOL	CASE 301	515-1	511-10
10 kpsi	P_1	20.04	19.7	19.95
10 kpsi	P_2	4.146	33.3	3.998
sec	t_1	.057	.0568	.0568
sec	t_2	.056	.0564	.0565
sec	t_3	.0557	.0558	.0558
sec	σ_1	.0027	.00279	.00270
sec	σ_2	.00051	.000597	.000519
Hz	f	327.6	344.4	361.08
No of Iterations		18	19	21
Computing Time (sec)		51.2	58.0	63.2
Experimental Variance (σ_e^2)		NOT APPLICABLE	$(.45)^2$	$(.317)^2$

TABLE 1. Parameters Fitting Pressure Curve.

CASE ORDER	301	511-5	511-10
1	.717	.680	.696
2	.477	.427	.443
3	.286	.247	.248
4	.058	.027	.013
5	-.113	-.136	-.160
6	-.246	-.258	-.291
7	-.303	-.315	-.346
8	-.322	-.334	-.361
9	-.307	-.312	-.342
10.	-.245	-.240	-.276
11.	-.130	-.104	-.155
12.	-.011	.031	-.035
13.	.069	.130	.048
14.	.137	.217	.123
15.	.110	.203	.106
16.	.075	.168	.085
17.	-.028	.057	.0004
18.	-.141	-.068	-.090
19.	-.202	-.149	-.130
20.	-.235	-.205	-.145
Sum. Sqs.	57.9	67.9	57.62
χ_1^2	57.9	62.96	116.2
χ_2^2	-	33.01	62.4
χ_{TOT}	-	95.97	178.6

Table 2. Autocorrelations and Chi-Square for final model of XM211 Pressure Oscillations. (χ_2^2 based on the first 5 Autocorrelations for Case 511-5, and the first 10, for case 511-10)

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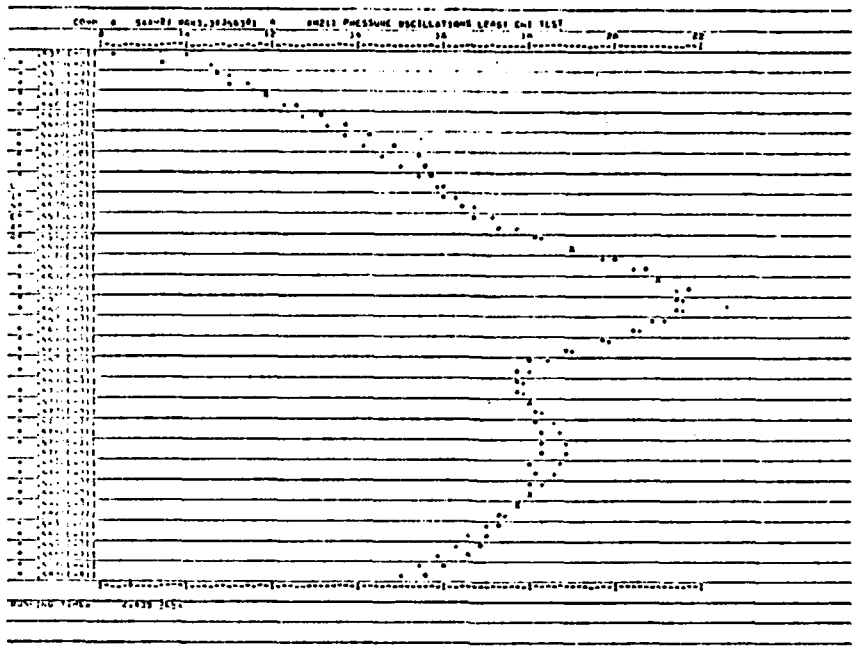

Figure 1 - Pressure as a function of time. "+"s indicate theory for case 301.

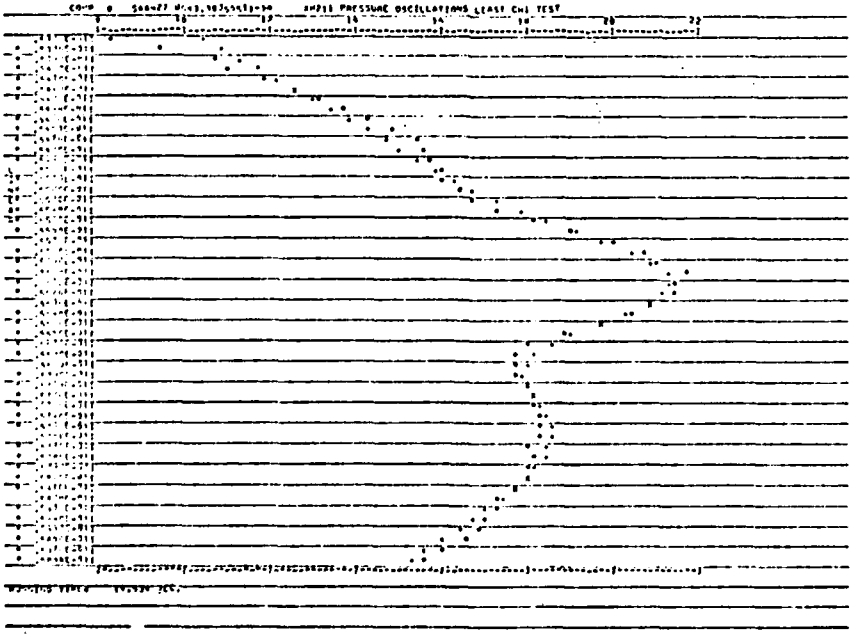

Figure 2 - Pressure as a function of time. "+"s indicate theory for case 511-5

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CASE	4.012-0	4.011-6
NO. of ITER.	4	2
L(0,4)	17.70	18.58
L(4,1)	53.11	53.02
L(4,2)	1.094	0.605
L(4,3)	6.204	10.26
R(I) 1		-.110
2		-.232
3		-.014
4		.068
5		-.124
6		.030
Sum of sqs	.03147	.03138
X_1^2	28.90	28.82
X_2^2	2.77	2.49
X_T^2	31.67	31.31

Table 3. Results of Yaw Damper Calculations

ITEM/CASE	KJE 1.0021-0	KJE 1.0023-5
L(1,2)	.2155	.2199
L(2,1)	.4527	.4442
L(3,1)	.0431	.0431
L(4,1)	.0252	.0251
L(5,1)	.0743	.0824
R(1)	.122	-.086
R(2)	.065	-.052
R(3)	.009	.034
R(4)	.227	-.223
R(5)	.179	-.168
X_1^2	31.22	31.24
X_2^2	3.99	3.04
X_{TOT}	35.21	34.28

Table 4. Results of Brookhaven example calculation. Autocorrelation, X_2, and X_T^2 for case KJE 1.0021-0 computed for comparison.

ITEM/CASE	KWB 1.003-0	KWB 1.005-3	KWB 1.0007-6
L(11,1)	5.318×10^{-4}	5.3183×10^{-4}	5.262×10^{-4}
R(1)	.782	.782	.786
R(2)	.44	.44	.453
R(3)	.098	.098	-.122
R(4)	-.204	-	-.170
R(5)	-.316	-	-.274
R(6)	-.235	-	.290
X_1^2	121.14	1.2×10^9	121.89
X_2^2	36.71		35.0
X_I^2	157.85		156.89

Table 5. Results of Kinetic Experiment Water Boiler Calculations

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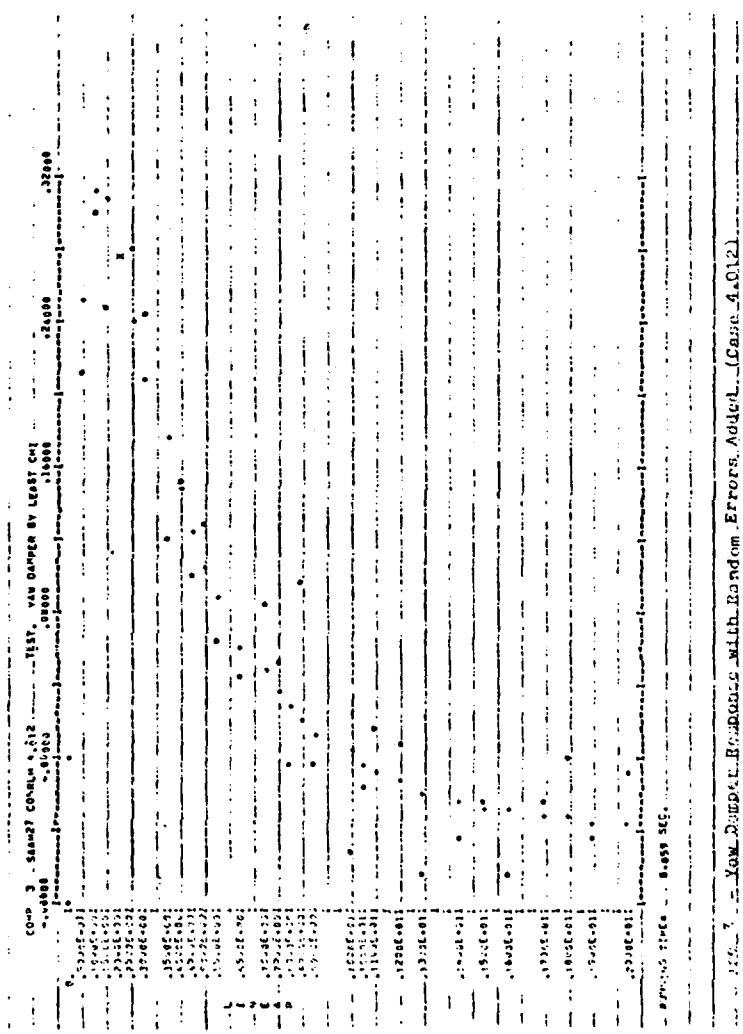

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The times for one iteration were 8.2 and 8.5 sec respectively. (Part of the increase in time for the least chi-square case was due to several attempts in both iterations to improve the fit by reducing the step size.) As shown in Table 3 the parameters L(0, 4), L(4,2) and L(4,3) appear to be different by significant amounts. (The autocorrelations for case 4.011-6 appear well within the random range.) The normalized sum of squares of the residuals is less, as expected, for the ordinary least squares, Case 4.012.

Brookhaven Example. A sample test case was received from Miss Rita Straub of Brookhaven National Laboratory. The exact nature of the probem was unspecified but from the form of the differential equations it appears to be a kinetic problem in which the material in component one decays into components two to five, and component two may change into component one. Component seven is composed of components three, four, and five. Although some coupling parameters may actually be unknown, they were assumed known, because the present version of the program will not iterate either type of linear coupling parameter with the least chi-square algorithm. The data were available for the amount of components 1, 3, 4, and 6 as a function of time, (where component 6 is the sum of components 1, 2, and 5).

Both the run with no autocorrelations and the run with 5 correlations (KJE 1.0023-5), took 7 iterations to converge. The results for the two cases are compared in Table 4. Since the value of X_1^2, (31.24) is large compared to X_2^2 (3.04), the major emphasis in this case was on reducing the sum of squares, and thus it is similar to the case run with no weight on the autocorrelations. As would be expected, there is only a small difference between the final values of the parameters of the two cases.

Reactor Kinetics Example. This example illustrates two things: First the use of the least chi-square algorithm, and second an apparently good fit between data and a physically incorrect model. Hetrick and Gamble (13) proposed a non-linear feed-back term proportional to the energy in the reactivity of the KEWB reactor to describe the fit. Later experiments (16) where the void amount was inferred from measurements and where the thermal effects on reactivity were also carefully measured, showed that shutdown was due to thermal, not void effects. In the simulation, the effect of the energy on void formation was simulated by the parameter L(11, 1). The functions correspond, in numerical order, to the functions used in the simulation: (1) Nuclear reactor power level, (2) Mean temperature, (3) Mean void volume, (4)-(9) Delayed neutron groups, (10) Not used, (11) Energy released to that time. The result of the iterations is shown in Figure 4, a logarithm plot of theoretical and experimental nuclear power. In Table 5, three different cases are shown:

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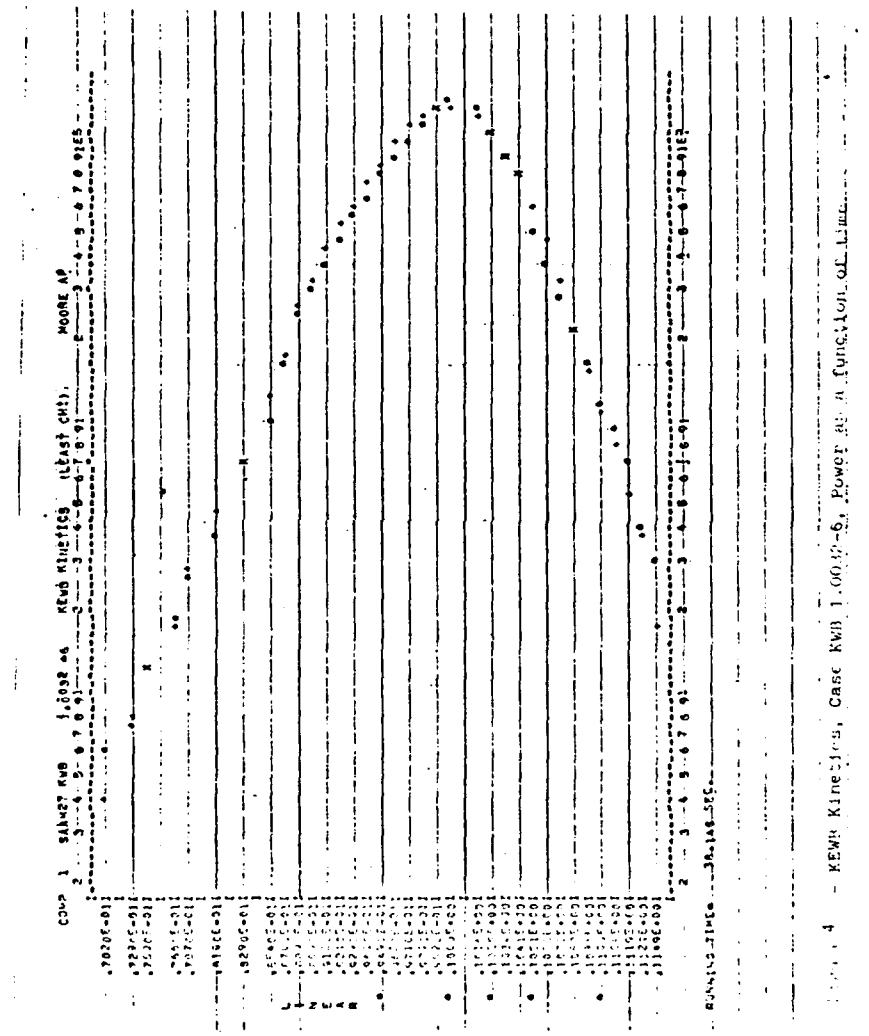

Figure 4 - KEWB Kinetics, Case KWB 1.00E-6, Power as a function of Time

Case 1.003-0 was ordinary least-squares. The values of the auto-correlations and chi-squares are shown for comparison with the other two cases. Case 1.005-3 used three autocorrelations with a small value of the experimental variance thus resulting in a large value of X_1^2. Both case 1.007-6 and 1.003-0 use 1×10^7 for the experimental variance thereby reducing the emphasis on the sum of the squares of the errors. All of these runs took four iterations to converge.

Cases 1.003-0 and 1.005-3 give almost exactly the same results. On comparing 1.003-0 with 1.007-6, a difference is found in the value of the adjustable parameter L(11,1). The value of chi-square total is smaller for 1.007-6, and thus this result would be chosen over that of the other case.

The value of the chi-square for the Box-Pierce number is much smaller for case 1.007-6, although X_1^2 is slightly larger for the same case--thus illustrating the trade-off between getting the minimum as in ordinary least squares, and reducing the autocorrelations as in least chi-squares. The data for Case 1.003 show the values for R(1) to R(6) for comparison purposes. The data show that the sum of squares does not increase from one to the other appreciably, but X_2^2, the Box-Pearce statistic, does change appreciably. Each of the calculations give a total chi square which is too large to be consistent with the residuals being drawn from a random sample, and thus would have given support for the rejection of the Hetrick-Gamble model.

Comparison of Computing Time. Table 6 summarizes the comparison of the number of iterations to converge, and the computing time. The number of iterations was usually about the same. As seen in the last column the computing time is comparable, with a tendency for the computing time to be longer for least chi-square than for least squares. The relative difference is greater when the original total computing time is short. This just means that, as would be expected, it takes a larger fraction of the computing time to compute the matrix Γ and post-multiply into P*' for cases where the time of iteration is short.

Conclusions. Based on four different types of non-linear theoretical models for data analysis, our results indicate that:

(1) Least chi-square is practicable for non-linear analysis.

(2) Least chi-square gives a better fit, and is a more reliable iteration procedure.

(3) The computing time for least chi-square is longer for the models which use less computing time, but because the convergence of this iterative procedure is somewhat better, the number of iterations (and particularly the number of "tries" per iteration) is reduced, thus keeping the total computing time about the same. Those models with longer integrating time would be expected to benefit more from least chi-square.

(4) In validation of simulations of future Army systems, the SAAM-27 computer program modified for least chi-square can be used at various stages in the system development. First, as a tool to simulate subsystems and compare the projected performance with the designer's simulation. Second, as subsystems are built and tested, they can be run as "hardware in the loop" and the test data used in the least chi-square program to validate the computer simulation and provide system parameter identification. Because no programming is needed to run SAAM-27 on a variety of problems, both the programming time and the elapsed time is greatly reduced.

By planning ahead to use SAAM in the validation of the subsystem modeling and providing the needed subsystem tests, a Program Manager can reduce the time and effort needed to validate the contractor's system simulation and will be able to give an impartial, knowledgeable, and timely evaluation of each system.

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Case	No. of Adjustable Parameters	Rank of Audo-correlation	No of Iterations	Time (sec)
Gun Chamber Pressure Curve.	8	0	18	51.2
	8	5	19	58.0
	8	10	21	63.7
Yaw Damper.	4	0	4	8.2
	4	6	2	8.5
Biomedical Test Case.	5	0	5	14.9
	5	5	5	15.2
	5	5	7	21.5
Reactor Kinetics Experiment.	1	0	4	84
	1	3	4	81
	1	6	4	89

Table 6. Comparison of computing time and number of iterations.

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